Supplementary Material
Superconductivity in functionalized niobium-carbide MXenes

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Bulk Nb_2CCl_2 structures with *P6₃mmc* and *P-3m1* symmetries

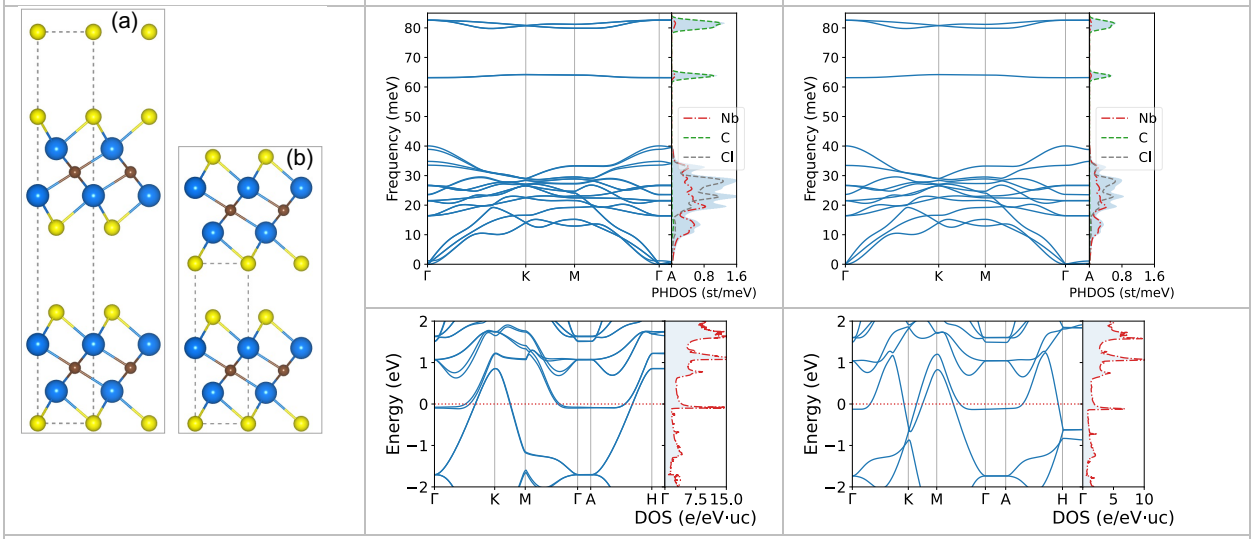


Figure S1: (a) Schematic representation of the periodic unit-cell of the Nb_2CCl_2 crystals with space group symmetries (a) *P6₃mmc* and (b) *P-3m1*. The calculated phonon dispersion along with phonon density of states, and electronic band structures of Nb_2CCl_2 crystals with space group symmetries (c) *P6₃mmc* and (d) *P-3m1*.

Exfoliation energies (E_x)

$E_x = (E_{Bulk} - n*E_{2D})/N$
E_{Bulk} = Total energy of the bulk structure
E_{2D} = Total energy of the single layer
n = Number of layers in the bulk unit cell
N = Number of atoms in the unit cell of the bulk structure

Note: Total energies were obtained using the PBE functional, without the inclusion of vdW interactions.

Materials	E_x (meV/Atom)
Nb_2CS_2	-1.08
Nb_2CCl_2	-1.03
$Nb_3C_2S_2$	-0.53
$Nb_3C_2Cl_2$	-0.52

Monolayer Nb_2CCl_2

Superconducting properties

***tsmear* = 0.0075 Ha μ^* = 0.13 Tc = 9.6 K**

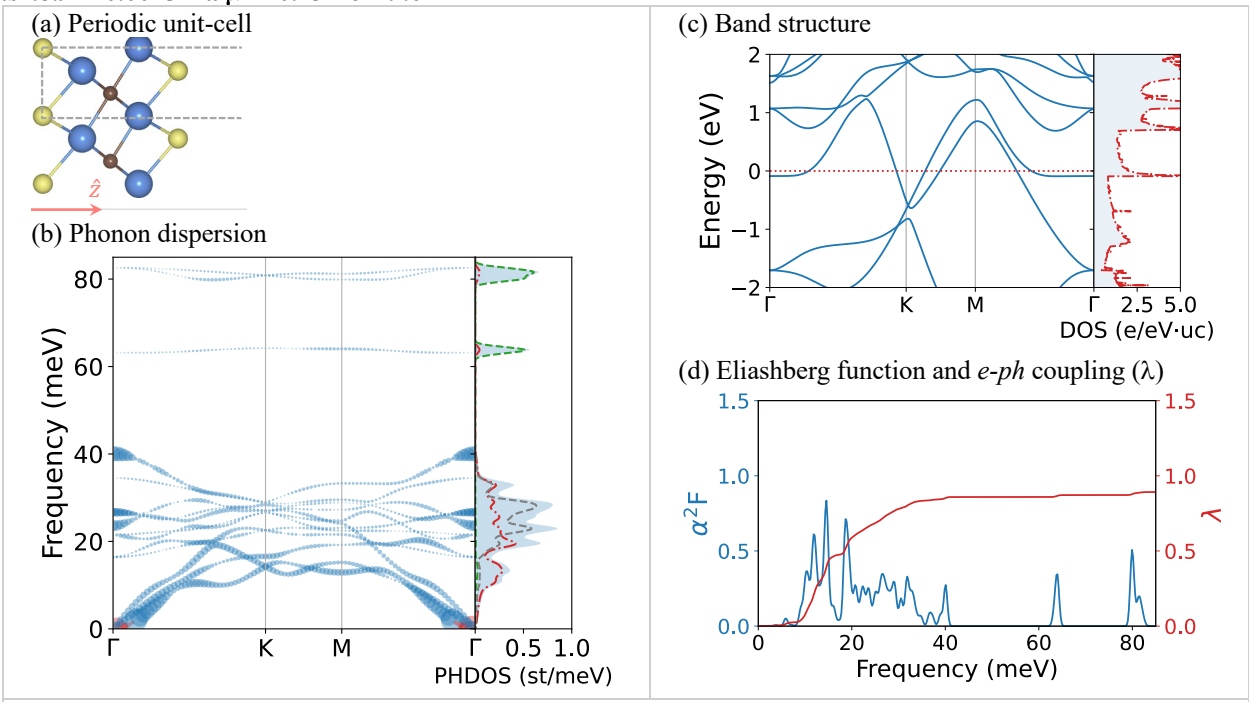


Figure S2: (a) Schematic representation of the periodic unit-cell of the considered crystal. The calculated (b) phonon dispersion along with *e-ph* coupling (size of red circles) and phonon density of states, (c) electronic band structure, and (d) Eliashberg function and integrated *e-ph* coupling constant (λ). The size of red circles is scaled with 1/100 for a better view. Here the red, grey, and green lines correspond to the Nb, Cl, and S atoms, respectively.

Monolayer Nb_2CCl_2

The Fermi level dependent superconducting properties of monolayer Nb_2CCl_2

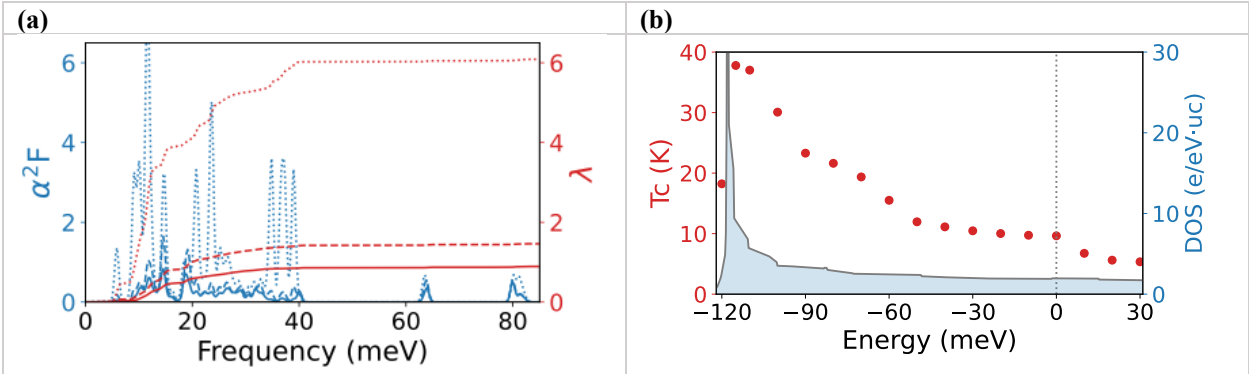


Figure S3: (a) Eliashberg function and integrated *e-ph* coupling constant for Fermi level shifted by gating to 0, -70, and -110 meV. (b) The calculated superconducting transition temperature T_c, along with electronic density of states at E_F.

Bulk-layered Nb_2CS_2

The calculated nesting function

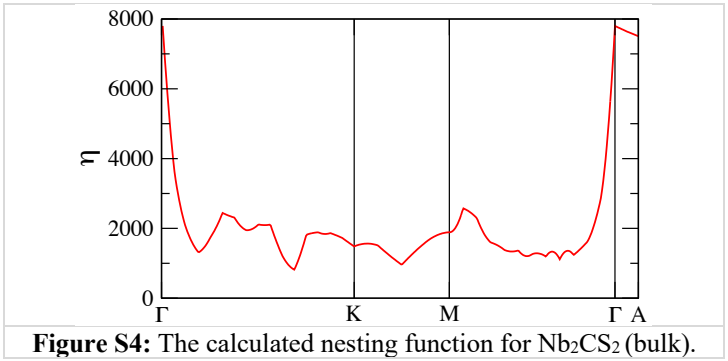


Figure S4: The calculated nesting function for Nb_2CS_2 (bulk).

Monolayer Nb_2CS_2

The change in Eliashberg function and integrated e-ph coupling constant (λ) with applied strain

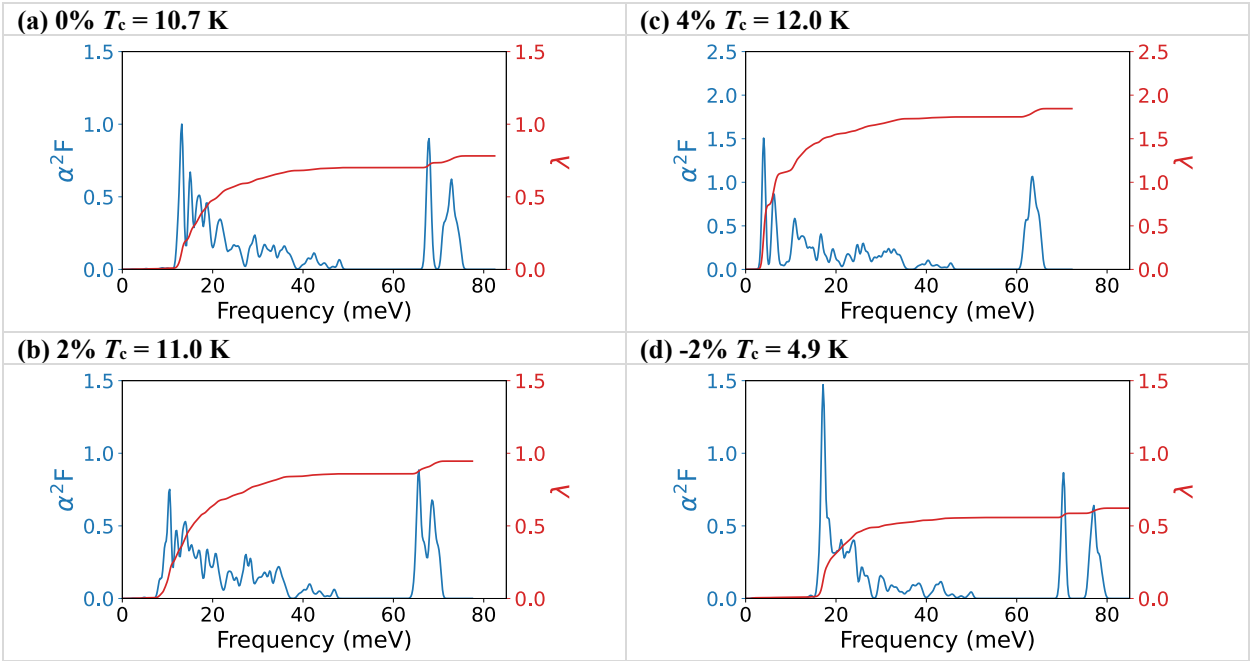


Figure S5: The calculated Eliashberg function and integrated e-ph coupling constant (λ) for different strain values (tensile (+) and compressive (-)). Here, $\mu^* = 0.13$ and *tsmear* = 0.005 Ha.

Bulk Nb_2CSe_2

Superconducting properties
***tsmear* = 0.0015 Ha T_c = 0.0 K**

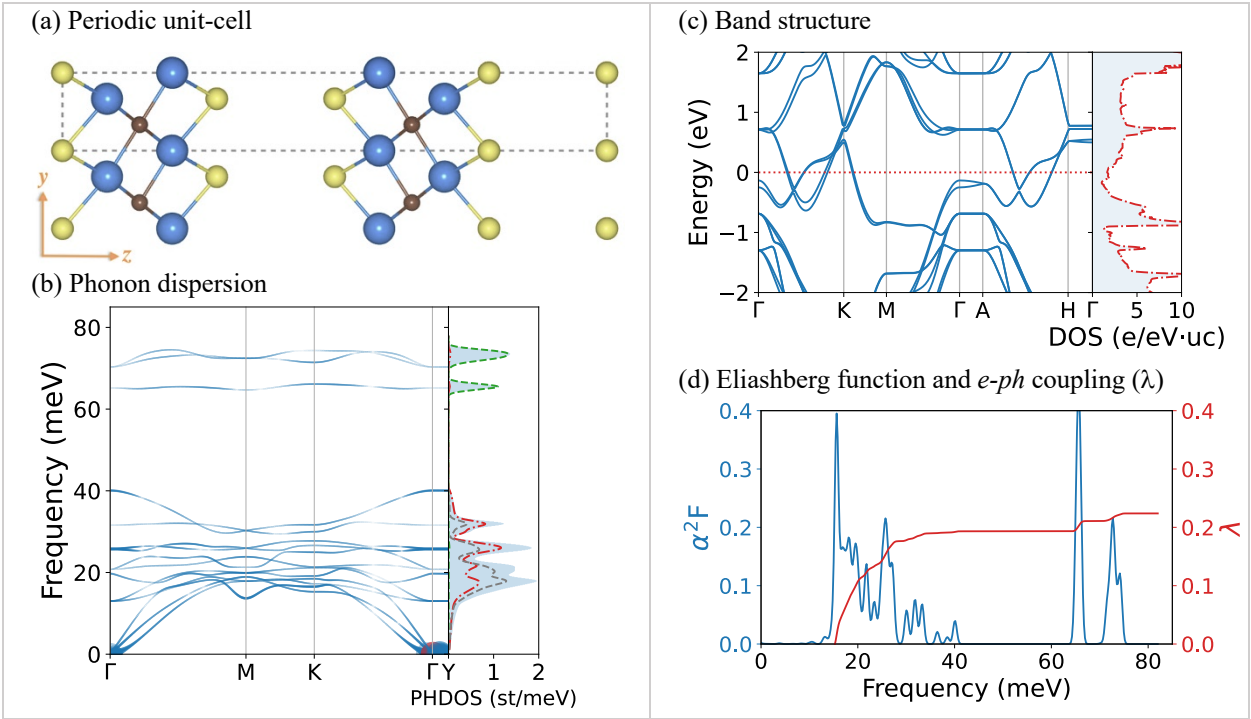


Figure S6: (a) Schematic representation of the periodic unit-cell of the considered crystal. The calculated (b) phonon dispersion along with *e-ph* coupling (size of red circles) and phonon density of states, (c) electronic band structure, and (d) Eliashberg function and integrated *e-ph* coupling constant (λ). The size of red circles is scaled with 1/100 for a better view. Here the red, grey and green lines correspond to the Nb, Se, and C atoms, respectively.

Monolayer Nb_3C_2

Superconducting properties
***tsmear* = 0.010 Ha T_c = 1.0 K**

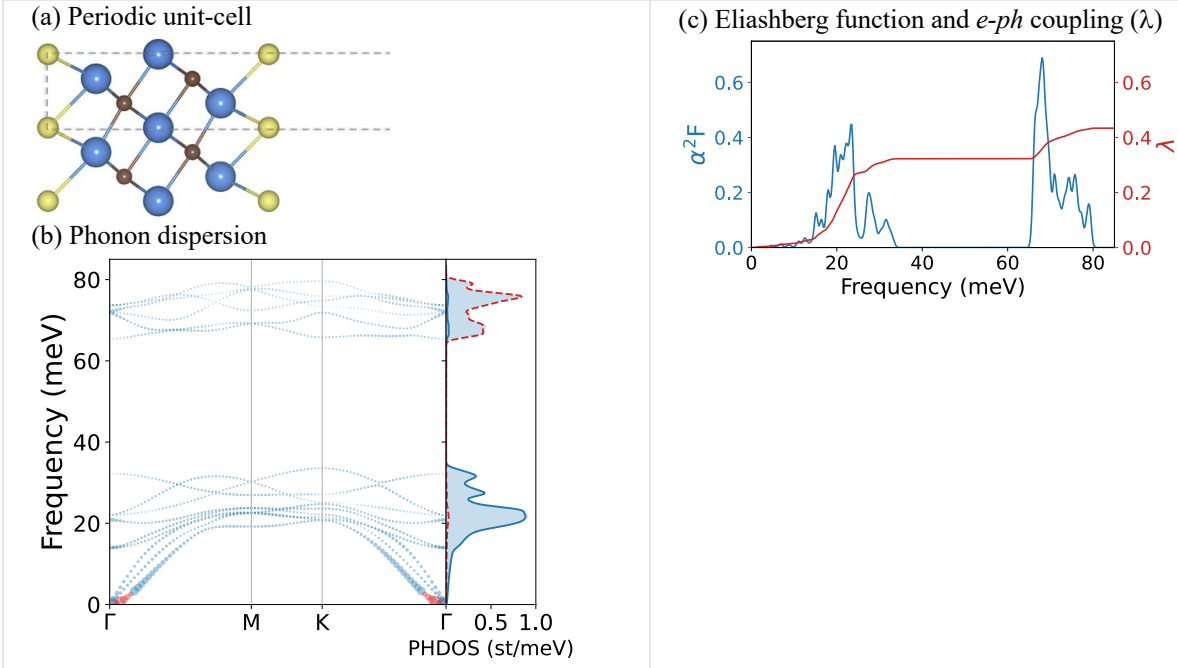


Figure S7: (a) Schematic representation of the periodic unit-cell of the considered crystal. The calculated (b) phonon dispersion along with *e-ph* coupling (size of red circles) and phonon density of states, and (c) Eliashberg function and integrated *e-ph* coupling constant (λ). The size of red circles is scaled with 1/100 for a better view. Here the blue, and red lines correspond to the Nb, and C atoms.

Bulk $Nb_3C_2Cl_2$
Space group *P-3m1*

Phonon dispersion
***tsmear* = 0.0075 Ha**

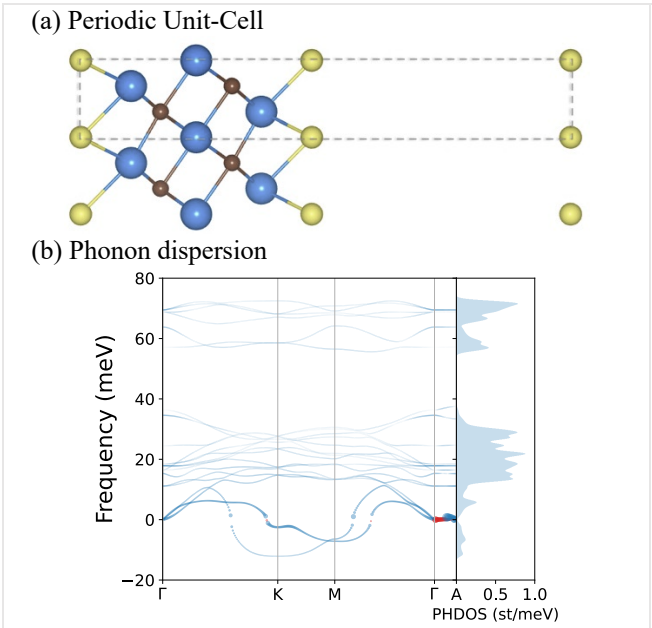


Figure S8: (a) Schematic representation of the periodic unit-cell of the considered crystal. (b) The calculated phonon dispersion along with *e-ph* coupling (size of red circles) and phonon density of states.

Monolayer $Nb_3C_2S_2$

Superconducting properties
***tsmear* = 0.0050 Ha T_c = 28.1 K**

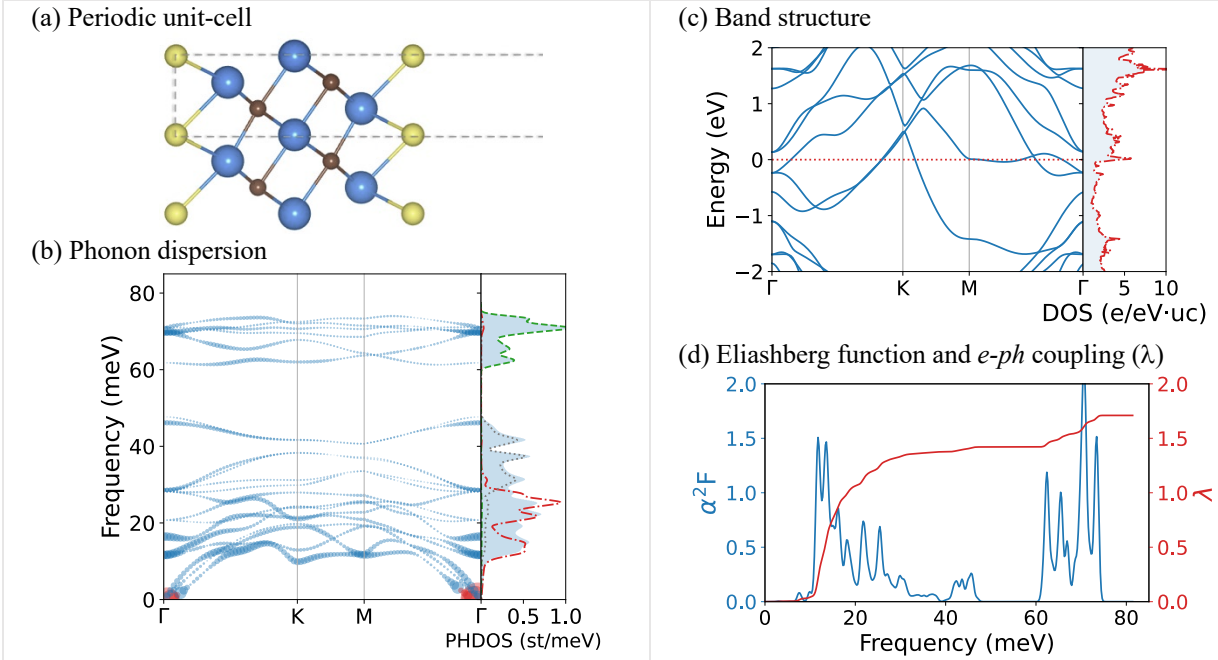


Figure S9: (a) Schematic representation of the periodic unit-cell of the considered crystal. The calculated (b) phonon dispersion along with *e-ph* coupling (size of red circles) and phonon density of states, (c) electronic band structure, and (d) Eliashberg function and integrated *e-ph* coupling constant (λ). The size of red circles is scaled with 1/10 for a better view. Here the red, grey and green lines correspond to the Nb, S, and C atoms, respectively.

Bulk Nb_2CCl_2

The calculated electronic density of states and carrier doping level

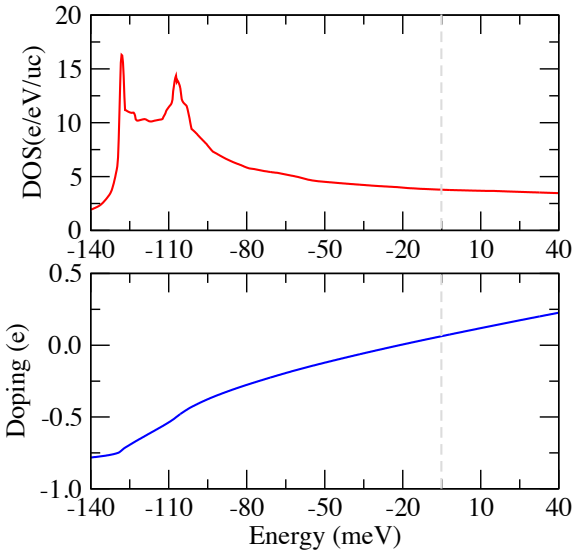


Figure S10: The calculated electronic density of states and corresponding electron doping for bulk Nb_2CCl_2. Here, the Fermi level is set to 0 eV.

Monolayer Nb_2CCl_2

The calculated electronic density of states and carrier doping level

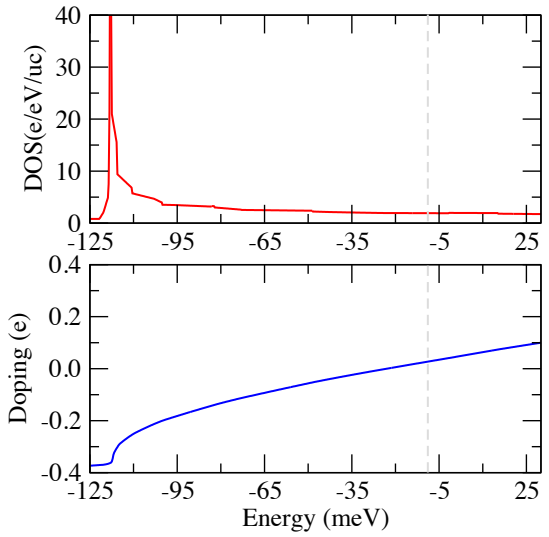


Figure S11: The calculated electronic density of states and corresponding electron doping for monolayer Nb_2CCl_2. Here, the Fermi level is set to 0 eV.

Monolayer Nb_2CCl_2

The change in band structure with tensile strain

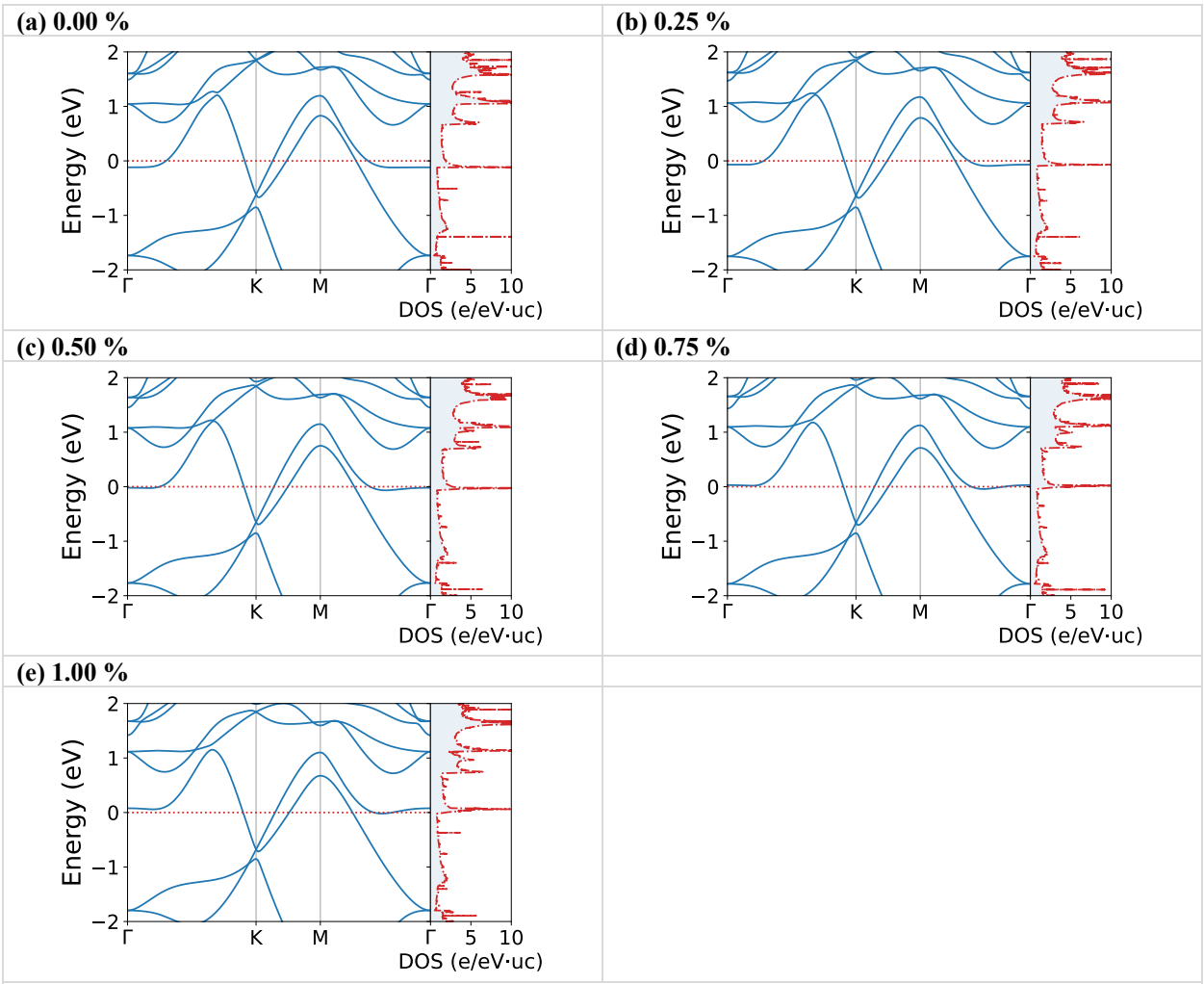
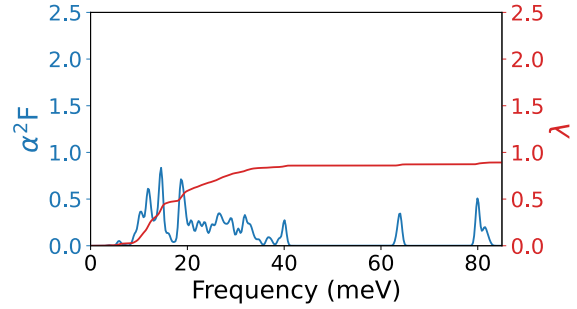


Figure S12: The calculated band structures for different tensile strain values.

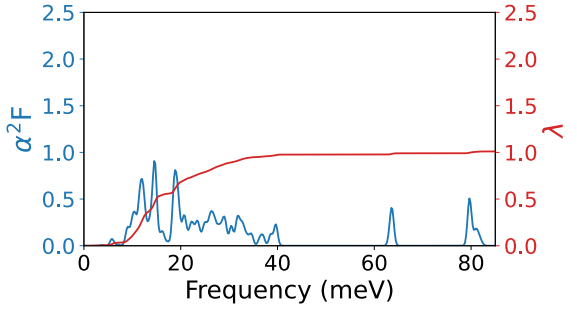
Monolayer Nb_2CCl_2

The change in Eliashberg function and integrated e-ph coupling constant (λ) with tensile strain

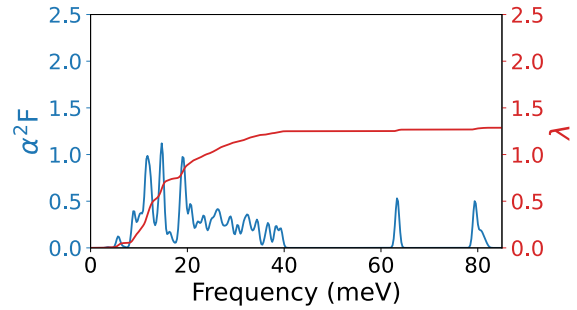
(a) 0.00 % T_c = 10.5 K



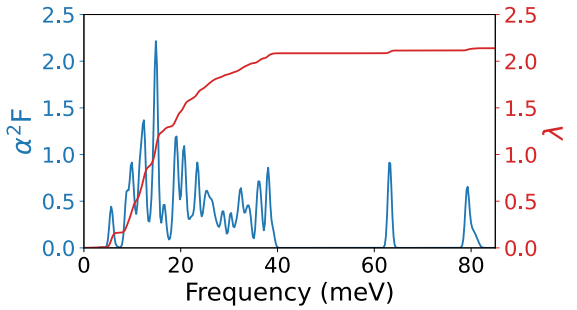
(b) 0.25 % T_c = 11.8 K



(c) 0.50 % T_c = 16.4 K



(d) 0.75 % T_c = 25.6 K



(e) 1.00 % T_c = 4.3 K

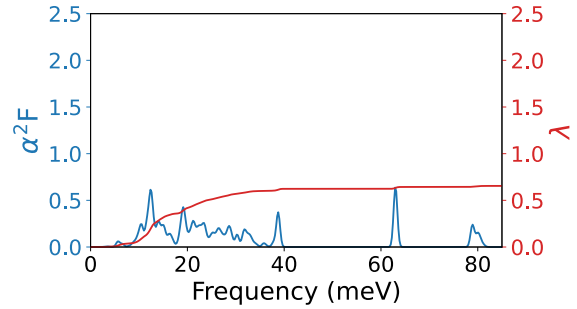


Figure S13: The calculated Eliashberg function and integrated e-ph coupling constant (λ) for different tensile strain values. Here, μ^* = 0.13 and *tsmear* = 0.0075 Ha.

Monolayer Nb_2CCl_2

The change in phonon dispersion with tensile strain

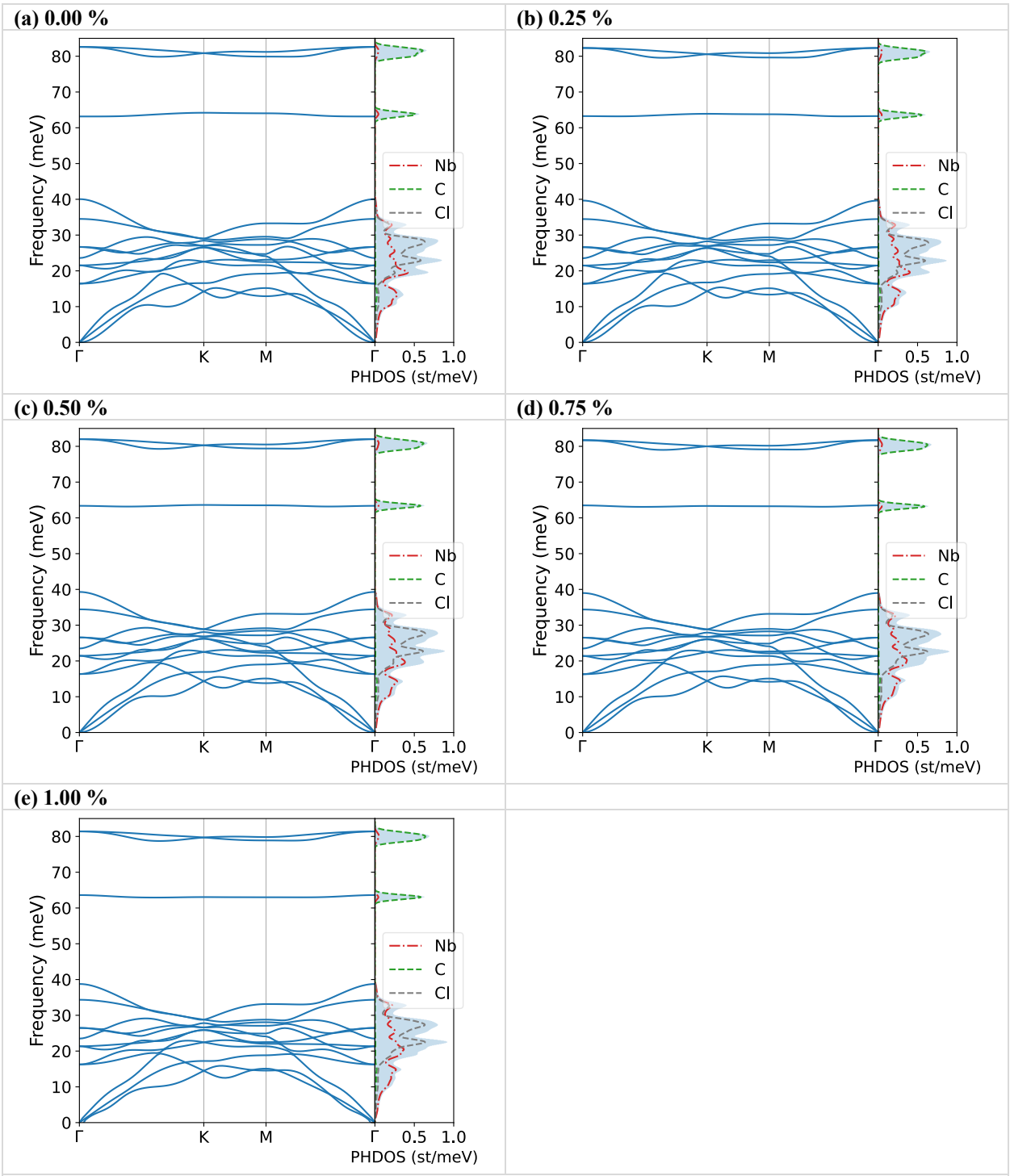


Figure S14: The calculated phonon dispersions for different tensile strain values.

Monolayer Nb_2CS_2

Superconducting properties
***tsmear* = 0.0015 Ha T_c = 10.7 K**

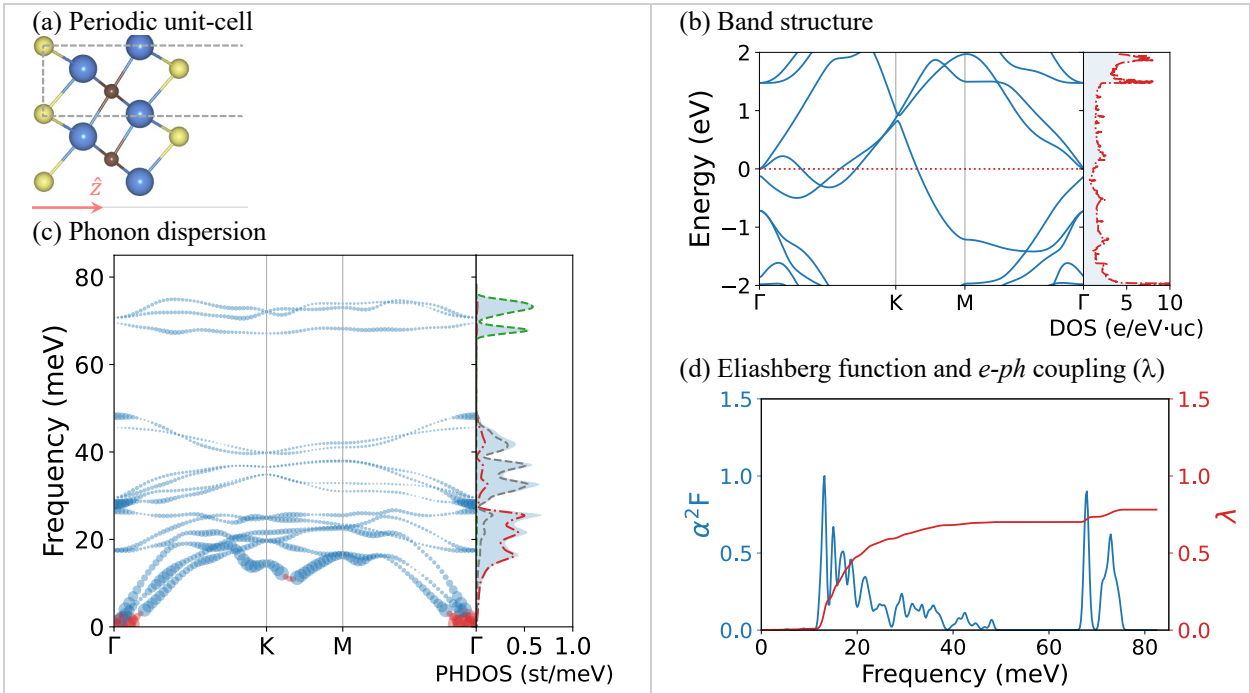


Figure S15: (a) Schematic representation of the periodic unit-cell of the considered crystal. The calculated (b) phonon dispersion along with *e-ph* coupling (size of red circles) and phonon density of states, (c) electronic band structure, (d) Eliashberg function and integrated *e-ph* coupling constant (λ). The size of red circles is scaled with 1/10 for a better view. Here the red, grey, and green lines correspond to the Nb, S, and C atoms, respectively.

Monolayer Nb_2CS_2

The change in band structure with applied strain

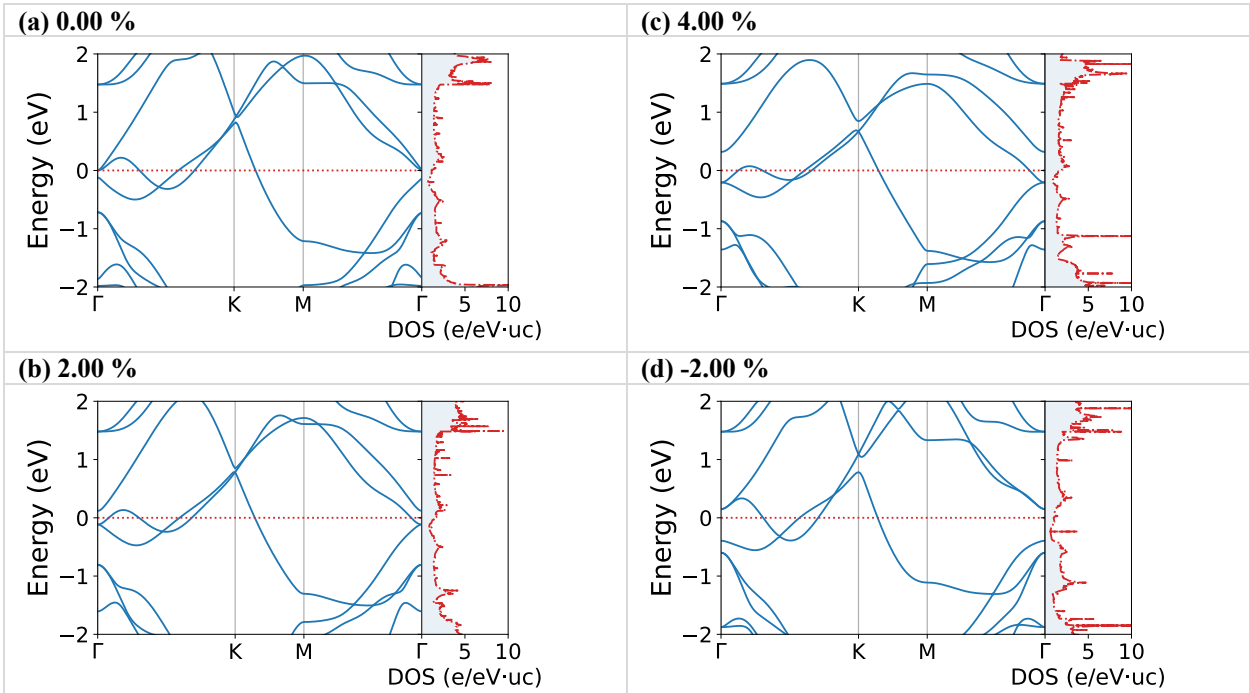


Figure S16: The calculated band structures for different strain values (tensile (+) and compressive (-)).

Monolayer Nb_2CS_2

The change in phonon dispersion with applied strain

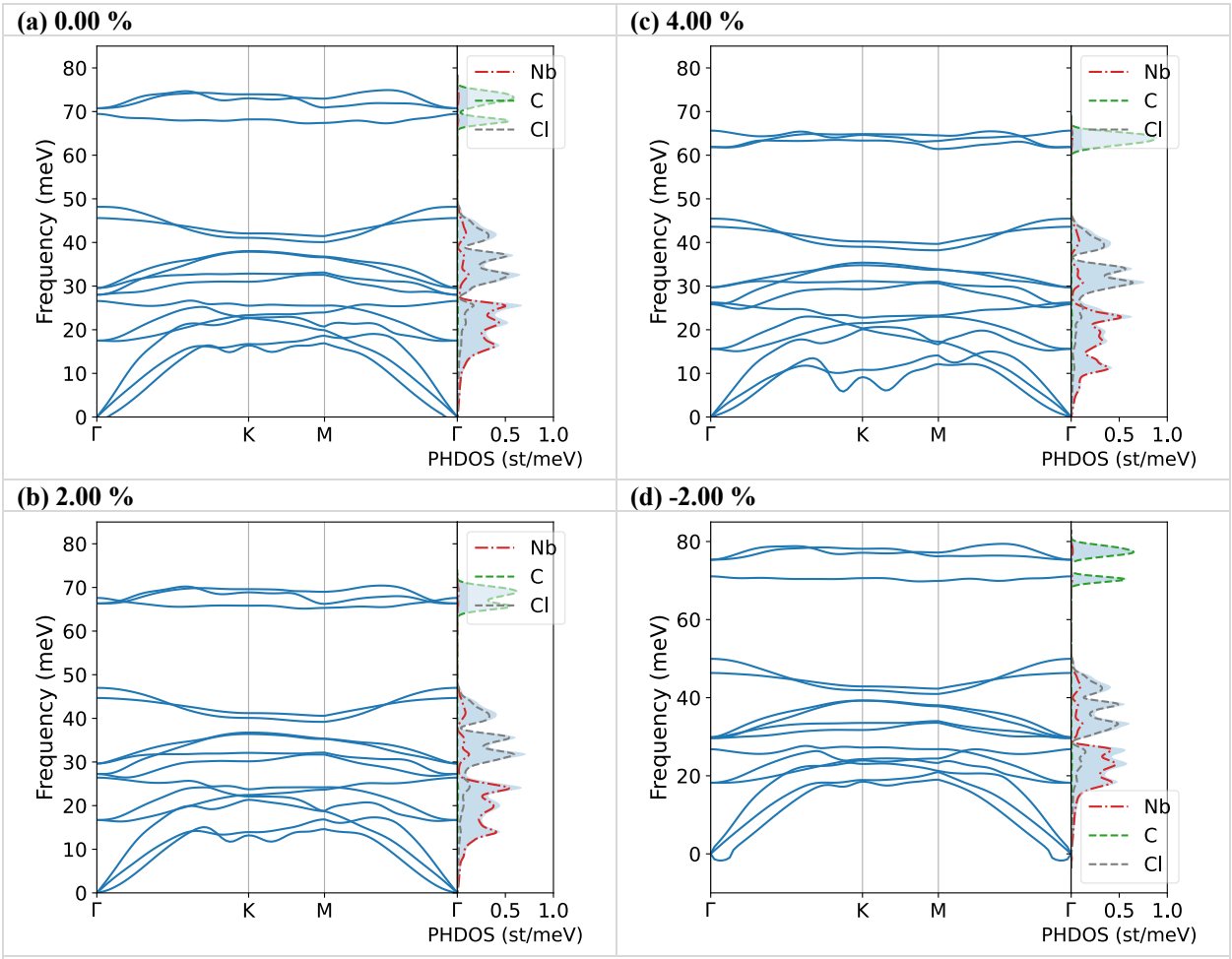


Figure S17: The calculated phonon dispersions for different strain values (tensile, + and compressive, -).

Monolayer Nb_2CS_2

The calculated nesting function

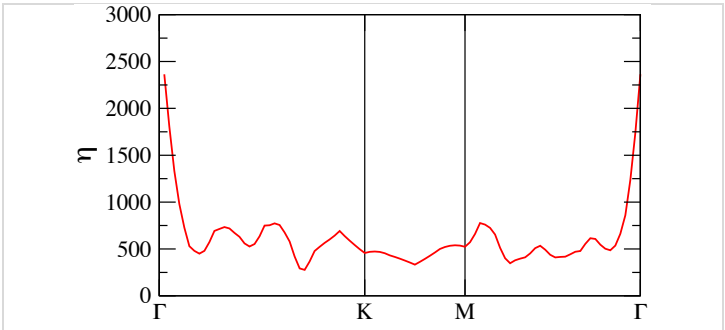


Figure S18: The calculated nesting function for Nb_2CS_2 (2D).